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Application of electric field to aluminum/copper/aluminum trilayer nanocomposites and determination of mechanical properties: A molecular dynamics approach

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Highlights

- Effects of EEF with different values on the mechanical properties of three-layer Al/Cu/Al-NCs were evaluated.
- Using the MD simulation approach and LAMMPS software.
- Ultimate strength and Young's modulus of designed samples decrease by EEF value enlarging.
- EEF is an important parameter in the mechanical evolution of MMNC structures.

Abstract

Most studies considered metal matrix nanocomposites (NCs) because of their excellent mechanical and electrical properties. In recent years, external electric fields (EEFs) in the aforementioned NCs were identified as a crucial role in modulating mechanical behavior. The EEF may affect strength, hardness, ductility, and fracture toughness. The explanation for these changes is the interaction of EEF with the nanoparticles in the metal matrix. In the present study, the effects of various EEF values on the mechanical properties of Al/Cu/Al three-layer NCs (TLNCs) were assessed using the molecular dynamics (MD) modeling method and LAMMPS software. MD findings predicted that the EEF reduced the physical stability and mechanical strength of modeled samples. Physically, this performance resulted from a decrease in attraction force among distinct particles inside the computing box in the presence of EEF. The proposed samples' ultimate tensile strength (UTS) and Young's modulus (YM) decreased to 2.587 GPa and 20.19 GPa, respectively, when the EEF value increased to 0.05 V/Å. Finally, it was determined that EEF is a crucial parameter in the mechanical development of MMNC structures and should be used in mechanical bacterial design in industrial applications.

Introduction

Metal matrix nanocomposites (MMNCs) were widely considered by most researchers due to having favorable mechanical and electrical properties [1], [2]. In recent years, the utilization of EFs in the NCs mentioned above was acknowledged as a critical factor in the further manipulation of the mechanical behavior. Research in this field demonstrated that the modification of EF effects on the mechanical properties of MMNCs can be conveyed in a variety of ways[3], [4], [5]. Understanding how EF affect these properties allows researchers to tailor materials for specific applications, leading to innovations in fields like robotics and smart materials [6], [7]. This research also contributed to fundamental knowledge about nanoscale phenomena, including charge carrier dynamics and interface behaviors, which are essential for developing next-generation materials [8], [9]. Surface bonds may be formed and altered by the EF by aligning particles and amplifiers. It may also have an effect on MMNC dislocation movement. Metal-based NCs with desired mechanical properties may be used in specialized applications including the electronics, automotive, and aerospace sectors using an EF [10], [11], [12], [13], [14].

For instance, Besharat et al. [15] investigated the alignment effects of graphene oxide (GO) nanosheets that were created due to the application of an EF in the polyether sulfone matrix. EFs were used alternately in each AC and DC mode, and the results were analyzed. The results indicate that GO/polyether sulfone NC was well aligned with GO nanosheets, and the nanoparticles were evenly disseminated throughout the matrix, with a GO concentration of approximately (0.02–0.1 % wt). Assume that the accumulation of nanosheets was facilitated by increased loadings (1 and 2 % wt). Furthermore, the tensile strength of investigated NC by the horizontal EF improved by 24 % compared to the vertical EF. Using DC EF, Jangam et al. [16] evaluated the effects of the alignment of multi-walled carbon nanotubes (MWCNT) in an epoxy matrix on the tensile fatigue performance of NCs. Different amounts of MWCNT (0.1, 0.2 and 0.3 wt%) were used in the NCs, and the tensile fatigue performance was determined using a sinusoidal load at a frequency of 1–3 Hz. The results of fatigue fracture were analyzed using the scanning electron microscope method. The results show that in low amounts of MWCNT (0.2 wt%), the fatigue life increased by approximately 13–15 %. Gao et al. [17] investigated the effect of alignment and dispersion of functionalized CNTs caused by the application of AC EF on the properties of natural rubber. The results show that MWCNTs aligned by EF had a more advantageous orientation and uniform dispersion than MWCNTs that were randomly distributed. Additionally, NC aligned using an EF had a thermal conductivity that was 8.67 % greater than those using random MWCNTs. Besides, aligned NCs had better mechanical properties than NC with random MWCNTs. Yakovenko et al. [18] evaluated the electrical properties of composite materials reinforced with carbon nanoparticles. An AC EF was used to align the carbon nanoparticles in the epoxy matrix. Additionally, the electrical properties of composite materials reinforced with carbon nanoparticles were assessed by this research group. An AC EF was used to align the carbon nanoparticles in the epoxy matrix. The results indicate that using EF resulted in an increase and enhancement of the alignment of carbon nanoparticles in composite materials, which led to an increase in electrical conductivity. Besides, using EF and alignment reduced the penetration threshold. Therefore, it is important to create alignment by the EF to create the desired conductivity.

Using a DC EF, Masraff et al. [19] investigated the effects of the alignment of silver nanoparticles in polydimethylsiloxane composite and its effects on thermal conductivity. Using an EF between 3.3 kV/cm and 10 kV/cm allowed the required nanoparticles to align, and the result was a 95 % increase in electrical conductivity in the longitudinal direction relative to the lateral direction. Huo et al. [20] evaluated the physical aging process of PMMA- TiO_2 NCs using an external EF. Using the EF, the alignment of the particles was done. The results indicate that the aging rate of material increased as a result of the addition of TiO_2 nanoparticles with random dispersion, while the aging rate decreased significantly as a result of the nanoparticles' alignment. Chen et al. [21] investigated the fracture toughness of sodium nanowire/epoxy titanate ($Na_2Ti_6O_{13}$) NCs using DC EF. The research findings indicated that the fracture strength of desired NC and 0.5 wt% nanowires increased by 11 % in comparison to pure epoxy when the nanowires were aligned perpendicular to the EF directions. In comparison to non-aligned samples, the alignment of NCs led to an 87 % increase in fracture strength. It is anticipated that the potential of metal matrix NCs to be utilized in the design and engineering of advanced materials will be demonstrated by examining the effect of the EF on their mechanical properties. Le et al. [22] focused the thermal properties of n-Hexacosane, a cost-effective phase-change material (PCM), using MD simulation. This study revealed that increasing the initial temperature enhances thermal conductivity and heat transfer, thereby improving the material's total thermal performance. Amendola et al. [23] focused the modelling of the mechanical behavior of biomaterials which are often reinforced by collagen and elastin fibers, leading to significant dispersion and anisotropy. In an effort to better understand the mechanical reactions of fiber-reinforced soft tissues, this research presented a new model for anisotropic dispersion in transversely isotropic materials.

The research that was conducted thus far was not examined the effect of EF on the mechanical properties of metal NCs. Consequently, the mechanical properties of Al/Cu/Al-TLNCs were assessed using the MD simulation approach and LAMMPS software in the current study, which examined the effect of EF with various values. For this purpose, the change in the stress-strain curve, YM, UTS were investigated. This study had broader implications for material design and optimization. By evaluating the stress-strain behavior under varied EF circumstances, researchers may determine ideal configurations for certain applications, opening the path for the creation of new materials with customizable mechanical properties. This understanding might have a huge effect on sectors that use high-performance materials, such as aerospace, automotive, and electronics. Ultimately, this research contributed to the advancement of nanotechnology and materials science by providing a foundational understanding of how external stimuli, like EFs, can be utilized to manipulate and enhance the properties of MMNCs.

Section snippets

Simulation approach

Computer simulation is a highly suitable and efficient approach for studying the structure and behavior of materials. Researchers showed a great deal of interest in the MD simulation among other computer simulation methods for figuring out the macroscopic properties of particulate systems because of its affordability, accuracy in modeling laboratory conditions, and user control[24], [25]. The MD method tracks the time-dependent behavior of system properties by analyzing microscopic …

Results

In the second phase of the current research, the mechanical properties of equilibrated Al-Cu-Al TLNC was reported. This process is implemented in the presence of EEFs. In the pristine sample, the value of EEF was set to 0.01 V/Å. As shown in Fig. 2, the physical stability can be detected in the atom-base system in the designed mechanical procedure. The stress-strain curve of Al-Cu-Al TLNC is shown in Fig. 6. During tensile testing, a sample was subjected to pulling forces that caused it to …

Conclusion

Mechanical performance of NC refers to the ability of these materials to withstand mechanical stresses and strains. NC are materials that consist of various nano-parts that are dispersed as a united sample. In current computational research, we described the mechanical performance of Al-Cu-Al trilayer NC (Al-Cu-Al TLNC) in the presence of an EFF by the MD approach. MD outputs predicted the physical stability of designed samples with kinetic and total energy convergence to 170.63 and …

Future suggestion

Here are some future research suggestions for exploring MMNCs:

- Explore the anisotropic nature of current material, focusing on its dispersive properties and how they affect mechanical performance under different loading conditions. …
- Study the effect of varying temperature conditions on the mechanical properties and stability of the NCs, particularly under extreme environments. …
- Research methods to optimize the distribution and alignment of nanoparticles within the matrix to enhance mechanical and …

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Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper. …

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